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NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JAN 02	STN pricing information for 2008 now available
NEWS	3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	5	JAN 28	MARPAT searching enhanced
NEWS	6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	8	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS	9	FEB 08	STN Express, Version 8.3, now available
NEWS	10	FEB 20	PCI now available as a replacement to DPCI
NEWS	11	FEB 25	IFIREF reloaded with enhancements
NEWS	12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS	14	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	16	MAR 31	CA/Caplus and CASREACT patent number format for U.S. applications updated
NEWS	17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	21	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS	22	APR 28	IMSRESEARCH reloaded with enhancements
NEWS	23	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS	24	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS EXPRESS	FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008		
NEWS HOURS	STN Operating Hours Plus Help Desk Availability		
NEWS LOGIN	Welcome Banner and News Items		
NEWS IPC8	For general information regarding STN implementation of IPC 8		

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 18:50:27 ON 04 JUN 2008

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 18:50:50 ON 04 JUN 2008  
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STRUCTURE FILE UPDATES: 3 JUN 2008 HIGHEST RN 1025148-33-7  
DICTIONARY FILE UPDATES: 3 JUN 2008 HIGHEST RN 1025148-33-7

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

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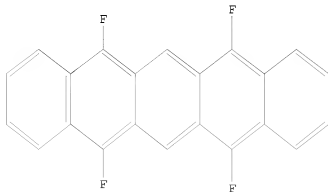
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdnoc/properties.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10578259-comp4.str

L1 STRUCTURE UPLOADED

=> d l1  
L1 HAS NO ANSWERS  
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 18:51:09 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 84 TO ITERATE

100.0% PROCESSED 84 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 1131 TO 2229

PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 18:51:13 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1679 TO ITERATE

100.0% PROCESSED 1679 ITERATIONS

13 ANSWERS

SEARCH TIME: 00.00.01

L3 13 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

178.36

178.57

FILE 'CAPLUS' ENTERED AT 18:51:18 ON 04 JUN 2008

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FILE COVERS 1907 - 4 Jun 2008 VOL 148 ISS 23

FILE LAST UPDATED: 3 Jun 2008 (20080603/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.

They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> s l3

L4 20 L3

=> d l4 ibib abs hitstr l-

YOU HAVE REQUESTED DATA FROM 20 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2008:57960 CAPLUS

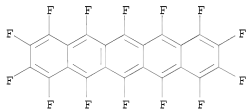
DOCUMENT NUMBER: 148:339532  
TITLE: Rational Design of Macrometallocyclic Trinuclear Complexes with Superior  $\pi$ -Acidity and  $\pi$ -Basicity  
AUTHOR(S): Tekarli, Sammer M.; Cundari, Thomas R.; Omary, Mohammad A.  
CORPORATE SOURCE: Department of Chemistry, Center for Advanced Scientific Computing and Modeling (CASCAM), University of North Texas, Denton, TX, 76203, USA  
SOURCE: Journal of the American Chemical Society (2008), 130(5), 1669-1675  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB D. functional theory (DFT) has been used to assess the  $\pi$ -acidity and  $\pi$ -basicity of metal-organic trimetallic macromol. complexes of the type  $[M(\mu-L)]_3$ , where  $M = Cu, Ag$ , or  $Au$  and  $L =$  carbeniate, imidazolate, pyridinate, pyrazolate, or triazolate. The organic compds. benzene, triazole, imidazole, pyrazole, and pyridine were also modeled, and their substituent effects were compared to those of the coinage metal trimers. Our results, based on mol. electrostatic potential surfaces and pos. charge attraction energy curves, indicate that the metal-organic macromols. show superior  $\pi$ -acidity and -basicity compared to their organic counterparts. Moreover, the metal-organic cyclic trimers are found to exhibit  $\pi$ -acidity and -basicity that can be systematically tuned both coarsely and finely by judicious variation of the bridging ligand (relative  $\pi$ -basicity imidazolate > pyridinate > carbeniate > pyrazolate > triazolate), metal (relative  $\pi$ -basicity  $Au > Cu > Ag$ ), and ligand substituents. These computational findings are thus guiding exptl. efforts to rationally design novel  $[M(\mu-L)]_3$  materials for applications in mol. electronic devices that include metal-organic field-effect transistors and light-emitting diodes.

IT 646533-88-2  
RL: PRP (Properties)  
(rational design of macrometallocyclic trinuclear complexes with superior  $\pi$ -acidity and  $\pi$ -basicity)

RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



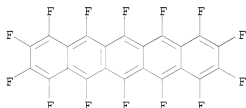
REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2007:1450340 CAPLUS  
DOCUMENT NUMBER: 148:152510  
TITLE: The lowest triplet electronic states of polyacenes and perfluoropolyacenes  
AUTHOR(S): Zhang, Xiuhui; Li, Qian-Shu; Xie, Yaoming; Schaefer, Henry F., III  
CORPORATE SOURCE: Institute for Chemical Physics, Beijing Institute of Technology, Beijing, 510631, Peop. Rep. China

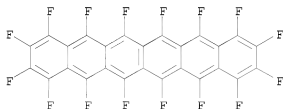
SOURCE: Molecular Physics (2007), 105(19-22), 2743-2752  
 CODEN: MOPHAM; ISSN: 0026-8976  
 PUBLISHER: Taylor & Francis Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The optimized geometries, total energies, and vibrational frequencies of the polyacenes and perfluoropolyacenes in their closed-shell singlet and lowest triplet states have been studied using the B3LYP method in conjunction with double- $\zeta$  plus polarization (DZP) basis sets. The equilibrium structures of all the polyacenes and perfluoropolyacenes are planar, with D<sub>2h</sub> symmetry, and the singlet and triplet geometries display interesting patterns for each family of mols. The largest singlet-triplet structural changes appear in the outermost C-C distances. The small perfluoropolyacene systems have ground state singlet states, and the singlet-triplet energy gaps decrease as the number of linearly fused benzene rings increases. With the number of rings greater than seven, the triplet state of the perfluorinated species falls below the closed-shell singlet. For the parent polyacenes, the same shift occurs between n = 8 and n = 9. Correspondingly, the LUMO-HOMO gap for the singlet state decreases with increasing number of linearly fused perfluoro benzene rings. The predicted singlet-triplet seps. for the perfluorinated compds. range from 54 kcal mol<sup>-1</sup> (perfluoronaphthalene) to -7 kcal mol<sup>-1</sup> (n = 10).

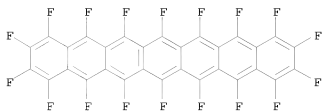
IT 646533-88-2 1001415-42-4 1001415-43-5  
 1001415-44-6 1001415-45-7 1001415-46-8  
 RL: PRP (Properties)  
 (lowest triplet electronic states of polyacenes and  
 perfluoropolyacenes)  
 RN 646533-88-2 CAPLUS  
 CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



RN 1001415-42-4 CAPLUS  
 CN Hexacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16-hexadecafluoro- (CA INDEX NAME)



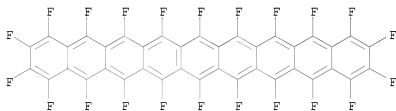
RN 1001415-43-5 CAPLUS  
 CN Heptacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18-octadecafluoro- (CA INDEX NAME)



RN 1001415-44-6 CAPLUS  
 CN Octacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20-eicosafuoro-  
 (CA INDEX NAME)



RN 1001415-45-7 CAPLUS  
 CN Nonacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22-  
 docosafuoro- (CA INDEX NAME)



RN 1001415-46-8 CAPLUS  
 CN Decacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24-  
 tetracosafuoro- (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2008 ACS ON STN  
 ACCESSION NUMBER: 2007:1379180 CAPLUS  
 DOCUMENT NUMBER: 148:154308  
 TITLE: Optical properties of pentacene and perfluoropentacene  
 thin films

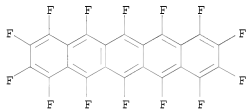
AUTHOR(S): Hinderhofer, Alexander; Heinemeyer, Ute; Gerlach, Alexander; Kowarik, Stefan; Jacobs, Robert M. J.; Sakamoto, Youichi; Suzuki, Toshiyasu; Schreiber, Frank  
CORPORATE SOURCE: Institut für Angewandte Physik, Universität Tübingen, Tübingen, 72076, Germany  
SOURCE: Journal of Chemical Physics (2007), 127(19), 194705/1-194705/6  
CODEN: JCPSA6; ISSN: 0021-9606  
PUBLISHER: American Institute of Physics  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The optical properties of pentacene (PEN) and perfluoropentacene (PFP) thin films on various SiO<sub>2</sub> substrates were studied using variable angle spectroscopic ellipsometry. Structural characterization was performed using x-ray reflectivity and atomic force microscopy. A uniaxial model with the optic axis normal to the sample surface was used to analyze the ellipsometry data. A strong optical anisotropy was observed, and enabled the direction of the transition dipole of the absorption bands to be determined. Also, comparison of the optical constants of PEN and PFP thin films with the absorption spectra of the monomers in solution shows significant changes due to the crystalline environment. Relative to the monomer spectrum, the HOMO to LUMO transition observed in PEN (PFP) thin film is reduced by 210 meV (280 meV). A 2nd absorption band in the PFP thin film shows a slight blueshift (40 meV) compared to the spectrum of the monomer with its transition dipole perpendicular to that of the 1st absorption band.

IT 646533-88-2, Perfluoropentacene  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)  
(optical properties of pentacene and perfluoropentacene thin films)

RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1018582 CAPLUS

DOCUMENT NUMBER: 147:352971

TITLE: Light emitting element, light emitting device, and electronic device

INVENTOR(S): Ohsawa, Nobuharu; Seo, Satoshi

PATENT ASSIGNEE(S): Semiconductor Energy Laboratory Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 46pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

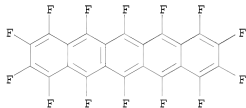
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 1833104 A2 20070912 EP 2007-4805 20070308  
 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,  
 IS, IT, LI, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR,  
 AL, BA, HR, MK, YU  
 KR 2007092135 A 20070912 KR 2007-22193 20070306  
 US 20070210322 A1 20070913 US 2007-715145 20070307  
 JP 2007273969 A 20071018 JP 2007-56525 20070307  
 CN 101034736 A 20070912 CN 2007-10085863 20070308  
 PRIORITY APPLN. INFO.: JP 2006-61969 A 20060308  
 AB Light-emitting elements comprising a first electrode; a second electrode;  
 and a first layer containing a light emitting substance interposed between the  
 first electrode and the second electrode are described in which the first  
 layer comprises a light emitting layer; a second layer containing a first  
 organic  
 compound; and a third layer containing a second organic compound, the first  
 electrode  
 has a light-transmitting property, the second layer and the third layer  
 are interposed between the second electrode and the light emitting layer,  
 and the colors of the first organic compound and the second organic compound  
 are  
 complementary. The first organic compound may have an absorption peak in the  
 wavelength region 380-540 nm, and the second organic compound in the wavelength  
 region 540-760 nm. Devices employing specific combinations of compds. are  
 described. Light-emitting devices employing the elements and electronic  
 devices with displays employing the light-emitting devices are also  
 described.  
 IT 646533-88-2, Perfluoropentacene  
 RL: TEM (Technical or engineered material use); USES (Uses)  
 (light-emitting elements with organic layers with complementary colors and  
 light-emitting devices and electronic devices using them for displays)  
 RN 646533-88-2 CAPLUS  
 CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX  
 NAME)



L4 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2007:836677 CAPLUS  
 DOCUMENT NUMBER: 147:476391  
 TITLE: Optical properties of pentacene and perfluoropentacene  
 thin films  
 AUTHOR(S): Hinderhofer, Alexander; Heinemeyer, Ute; Gerlach,  
 Alexander; Kowarik, Stefan; Jacobs, Robert M. J.;  
 Sakamoto, Youichi; Suzuki, Toshiyasu; Schreiber, Frank  
 CORPORATE SOURCE: Institut fuer Angewandte Physik, Universitaet  
 Tuebingen, Tuebingen, 72076, Germany  
 SOURCE: Los Alamos National Laboratory, Preprint Archive,  
 Condensed Matter (2007) 1-6, arXiv:0707.3768v1  
 [cond-mat.soft], 25 Jul 2007  
 CODEN: LNCMFR  
 URL: [http://arxiv.org/PS\\_cache/arxiv/pdf/0707/0707.3768v1.pdf](http://arxiv.org/PS_cache/arxiv/pdf/0707/0707.3768v1.pdf)  
 PUBLISHER: Los Alamos National Laboratory



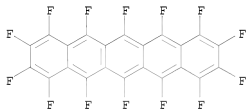
DOCUMENT TYPE: Preprint  
LANGUAGE: English

AB The optical properties of pentacene (PEN) and perfluoropentacene (PFP) thin films on various SiO<sub>2</sub> substrates were studied using variable angle spectroscopic ellipsometry. Structural characterization was performed using X-ray reflectivity and atomic force microscopy. A uniaxial model with the optic axis normal to the sample surface was used to analyze the ellipsometry data. A Strong optical anisotropy was observed and enabled the direction of the transition dipole of the absorption bands to be determined. Furthermore, comparison of the optical consts. of PEN and PFP thin films with the absorption spectra of the monomers in solution shows significant changes due to the crystalline environment. Relative to the monomer spectrum the HOMO-LUMO transition observed in PEN (PFP) thin film is reduced by 210 meV (280 meV). Surprisingly, a second absorption band in the PFP thin film shows a slight blueshift (40 meV) compared to the spectrum of the monomer with its transition dipole perpendicular to that of the first absorption band.

IT 646533-88-2, Perfluoropentacene  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)  
(optical properties of pentacene and perfluoropentacene thin films)

RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2007:678915 CAPLUS  
DOCUMENT NUMBER: 147:277260  
TITLE: 9,10-Dichlorooctafluoroanthracene as a Building Block for n-Type Organic Semiconductors  
AUTHOR(S): Tannaci, John F.; Noji, Masahiro; McBee, Jennifer; Tilley, T. Don  
CORPORATE SOURCE: Department of Chemistry, University of California at Berkeley, Berkeley, CA, 94720, USA  
SOURCE: Journal of Organic Chemistry (2007), 72(15), 5567-5573  
CODEN: JOCEAH; ISSN: 0022-3263  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 147:277260

AB 9,10-Dichlorooctafluoroanthracene (1) was synthesized from com. available tetrafluorophthalic acid by an optimized solution-phase route. To establish 1 as a synthon for n-type organic semiconductors, the compound was reacted with phenylboronic acid under modified Suzuki-Miyaura coupling conditions to generate octafluoro-9,10-diphenylanthracene (7) in 82% yield. Cyclic voltammetry and x-ray crystallog. indicate that 7 has a stabilized LUMO energy level and exhibits extended  $\pi$  stacking, which should lead to efficient electron transport in solid-state devices. 1,2,3,4,5,6,7,8-Octafluoroanthracene (2) was also synthesized as a potential n-type

building block, but suitable C-C coupling conditions for this compound were not found, and 2 could not be converted into 9,10-dibromooctafluoroanthracene or octafluoro-9,10-diiodoanthracene.

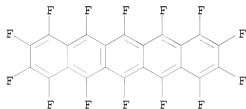
IT 646533-88-2, Perfluoropentacene

RL: PRP (Properties)

(preparation, structures and electronic properties of dichlorooctafluoroanthracene, diphenyloctafluoroanthracene and octafluoroanthracene via tetrafluorophthalic anhydride)

RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2007:660121 CAPLUS

DOCUMENT NUMBER: 147:266397

TITLE: Cyanation: providing a three-in-one advantage for the

design of n-type organic field-effect transistors

Kuo, Ming-Yu; Chen, Hsing-Yin; Chao, Ito

CORPORATE SOURCE: Institute of Chemistry, Academia Sinica Taipei, 11529, Taiwan

SOURCE: Chemistry--A European Journal (2007), 13(17), 4750-4758

CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The theor. work presented here demonstrates that, when substitution takes place at appropriate positions, cyanation could be a useful tool for reducing the internal reorganization energy of mols. A mol.-orbital-based explanation is given for this fundamentally important phenomenon. Some of the cyanated pentacene derivs. (nCN-PENT-n) not only have internal reorganization energies for electron transfer ( $\lambda^-$ ) smaller than that of pentacene, but the  $\lambda^-$  values are even of the same magnitude as the internal reorganization energy for hole transfer ( $\lambda^+$ ) of pentacene, a small value that few organic compds. have surpassed. In addition, cyanation raises the electron affinity of the parent compound and may afford good electronic couplings between neighboring mols., because of its ability in promoting  $\pi$ -stacking. For the design of high performance n-type organic field-effect transistors, high electron affinities, large intermol. electronic couplings, and small reorganization energies are necessary. Cyanation may help in all three aspects. Two cyanated trialkylsilylthynyl pentacene derivs. with known  $\pi$ -stacking structures are predicted to provide reasonably small internal reorganization energies, large electronic couplings, and high electron affinities. They have the potential to outperform N-fluoroalkylated dicyanoperylene-3,4;9,10-bis(-dicarboximides) (PDI-FCN2) in terms of electron mobility.

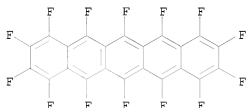
IT 646533-88-2, Perfluoropentacene

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(cyanation in preparation of materials for n-type organic field-effect transistors)

RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



REFERENCE COUNT: 73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:372393 CAPLUS

DOCUMENT NUMBER: 147:9534

TITLE: Effect of fluorination on the electronic structure and optical excitations of  $\pi$ -conjugated molecules

AUTHOR(S): Milian Medina, Begona; Beljonne, David; Egelhaaf, Hans-Joachim; Gierschner, Johannes

CORPORATE SOURCE: Laboratory for Chemistry of Novel Materials, Center for Research in Molecular Electronics and Photonics, University of Mons-Hainaut, Mons, 7000, Belg.

SOURCE: Journal of Chemical Physics (2007), 126(11), 111101/1-111101/6

CODEN: JCPSA6; ISSN: 0021-9606

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Fluorination of  $\pi$ -conjugated organic mols. is a strategy to obtain possible n-type conducting and air-stable materials due to the lowering of the frontier MOs (MOs) by the high electronegativity of fluorine. Nevertheless, the resulting optical gaps may be widened or narrowed, depending on the mol. backbone and/or the number and position of the fluorine atoms. The authors have performed time-dependent d. functional theory calcs. to address the subtle influence of fluorine substitution on the absolute MO energies and the subsequent impact on the optical transitions in homologous conjugated oligomers based on thiophene and acene units.

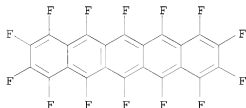
IT 646533-88-2

RL: PRP (Properties)

(effect of fluoro group substitution on electronic structure and optical excitations of  $\pi$ -conjugated mols.)

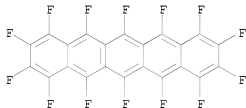
RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2007:175875 CAPLUS  
DOCUMENT NUMBER: 146:387992  
TITLE: The effect of fluorination on pentacene/gold interface energetics and charge reorganization energy  
AUTHOR(S): Koch, Norbert; Vollmer, Antje; Duhm, Steffen; Sakamoto, Youichi; Suzuki, Toshiyasu  
CORPORATE SOURCE: Institut fuer Physik, Humboldt-Universitaet zu Berlin, Berlin, 12489, Germany  
SOURCE: Advanced Materials (Weinheim, Germany) (2007), 19(1), 112-116  
CODEN: ADVMEW; ISSN: 0935-9648  
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Organic semiconductor/metal interface energetics play a key role in the performance of organic-based electronic devices. The comparative angle-resolved UPS (ARUPS) study of pentacene (PEN) and perfluoropentacene (PEP) on Au(111) reported here highlights the effect of perfluorination and mol. layer thickness on the interface energy.  
IT 646533-88-2, Perfluoropentacene  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)  
(effect of fluorination on pentacene/gold interface energetics and charge reorganization energy)  
RN 646533-88-2 CAPLUS  
CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)

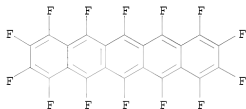


REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

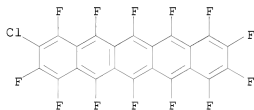
L4 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2007:60799 CAPLUS  
DOCUMENT NUMBER: 146:151909  
TITLE: Photoelectric element with high photoelectric efficiency containing halogenated pentacene, radiation image detector, and x-ray image-intensifier luminescent screen  
INVENTOR(S): Ozeki, Hidekane  
PATENT ASSIGNEE(S): Konica Minolta Medical & Graphic, Inc., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 47pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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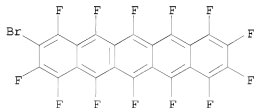
	JP 2007012982	A	20070118	JP 2005-193639	20050701
PRIORITY APPLN. INFO.:				JP 2005-193639	20050701
AB	Disclosed is a photoelec. element comprising a charge-generating layer, translucent electrode, and a counter electrode, wherein said charge-generating layer contains halogenated pentacene.				
IT	646533-88-2 919293-76-8 919293-77-9 919293-78-0				
	RL: TEM (Technical or engineered material use); USES (Uses) (charge-generating layer; Photoelec. element with high photoelec. efficiency containing halogenated pentacene for x-ray image-intensifier luminescent screen)				
RN	646533-88-2 CAPLUS				
CN	Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetrafluoro- (CA INDEX NAME)				



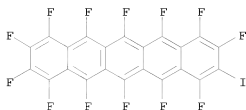
RN	919293-76-8 CAPLUS				
CN	Pentacene, 2-chloro-1,3,4,5,6,7,8,9,10,11,12,13,14-tridecafluoro- (CA INDEX NAME)				



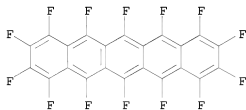
RN	919293-77-9 CAPLUS				
CN	Pentacene, 2-bromo-1,3,4,5,6,7,8,9,10,11,12,13,14-tridecafluoro- (CA INDEX NAME)				



RN	919293-78-0 CAPLUS				
CN	Pentacene, 1,2,3,4,5,6,7,8,9,11,12,13,14-tridecafluoro-10-iodo- (CA INDEX NAME)				



L4 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2006:88282 CAPLUS  
 DOCUMENT NUMBER: 145:177929  
 TITLE: Perfluoropentacene and Perfluorotetracene: Syntheses, Crystal Structures, and FET Characteristics  
 AUTHOR(S): Sakamoto, Youichi; Suzuki, Toshiyasu; Kobayashi, Masafumi; Gao, Yuan; Inoue, Youji; Tokito, Shizuo  
 CORPORATE SOURCE: Institute for Molecular Science, Myodaiji, Okazaki, Japan  
 SOURCE: Molecular Crystals and Liquid Crystals (2006), 444, 225-232  
 CODEN: MCLCD8; ISSN: 1542-1406  
 PUBLISHER: Taylor & Francis, Inc.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The syntheses and FET characteristics of perfluoropentacene and perfluorotetracene are described. Both acenes are planar and crystalline materials that adopt p-stack structures with the short interplanar distances of 3.27 Å in perfluorotetracene and 3.21 Å in perfluoropentacene. The oxidation and reduction peak potentials of the perfluorinated acenes shift pos. compared with those of the corresponding acenes, suggesting that the HOMO and LUMO energies are diminished by fluorine substituents. Organic field-effect transistors (OFETs) with perfluoropentacene exhibit n-type semiconducting properties with high electron mobility of 0.22 cm<sup>2</sup>/V s.  
 IT 646533-88-2P  
 RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)  
 (syntheses, crystal structures, and FET characteristics of perfluoropentacene and perfluorotetracene)  
 RN 646533-88-2 CAPLUS  
 CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)

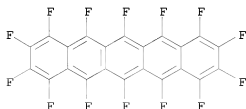


REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:903150 CAPLUS  
 DOCUMENT NUMBER: 143:239906  
 TITLE: Organic thin-film transistor, method for manufacturing

INVENTOR(S): same, and organic thin-film device  
Inoue, Youji; Tokito, Shizuo; Kobayashi, Masafumi;  
Gao, Yuan  
PATENT ASSIGNEE(S): Kanto Denka Kogyo Co., Ltd., Japan  
SOURCE: PCT Int. Appl., 43 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005078816	A1	20050825	WO 2005-JP2495	20050217
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
JP 2005235923	A	20050902	JP 2004-41397	20040218
GB 2426125	A	20061115	GB 2006-16379	20050217
KR 2007009564	A	20070118	KR 2006-716513	20060817
US 20070194302	A1	20070823	US 2006-589800	20060817
PRIORITY APPLN. INFO.:			JP 2004-41397	A 20040218
			WO 2005-JP2495	W 20050217
AB	Disclosed are an organic thin-film transistor with improved carrier mobility, a method for manufacturing an organic thin-film transistor, and an organic thin-film device comprising an organic thin-film transistor. Specifically disclosed is an organic thin-film transistor which comprises an organic semiconductor layer containing a fluorinated acene compound represented by the following formula: C <sub>4n+2</sub> F <sub>2n+4</sub> where n is an integer ≥ 2. The fluorinated acene compound may preferably be a tetradecafluoropentacene or a dodecafluoronaphthacene.			
IT	646533-88-2P, Perfluoropentacene RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses) (fluorinated acene thin-film transistor, method for manufacturing same, and organic thin-film device)			
RN	646533-88-2 CAPLUS			
CN	Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)			



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2005:697652 CAPLUS  
DOCUMENT NUMBER: 143:396162  
TITLE: Electron-phonon interactions in photoinduced excited electronic states in fluoroacenes  
AUTHOR(S): Kato, Takashi; Yamabe, Tokio  
CORPORATE SOURCE: Institute for Innovative Science and Technology, Graduate School of Engineering, Nagasaki Institute of Applied Science, Shuku-machi, Nagasaki, 851-0121, Japan  
SOURCE: Journal of Chemical Physics (2005), 123(2), 024301/1-024301/12  
CODEN: JCPSA6; ISSN: 0021-9606  
PUBLISHER: American Institute of Physics  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The electron-phonon coupling consts. [1Blu(HOMO LUMO)] in the photoinduced excited electronic states in fluoroacenes are estimated and compared with those in the monoanions (1LUMO) and cations (1HOMO). The 1Blu(HOMO LUMO) values are much larger than the 1LUMO and 1HOMO values in fluoroacenes. Furthermore, the Coulomb pseudopotential  $\mu^*$  values for the excited electronic states are estimated to be smaller than those for the monoanions and cations. The complete phase patterns difference between the highest occupied MOs (HOMOs) and the lowest unoccupied MOs (LUMOs) is the main reason why the electron-phonon coupling consts. and the  $\mu^*$  values are larger and smaller, resp., in the photoinduced excited electronic states than in the monoanions and cations. The possible electron pairing and Bose-Einstein condensation in the excited electronic states of fluoroacenes are discussed. Because of larger electron-phonon coupling consts. and smaller  $\mu^*$  values in the excited electronic states than in the charged states, the conditions under which the electron-electron interactions become attractive can be more easily realized, in principle, in the excited electronic states than in the charged states in fluoroacenes. The 1Blu(HOMO LUMO) values hardly change by H-F substitution, even though the 1LUMO and 1HOMO values significantly increase by H-F substitution in acenes. Antibonding interactions between carbon and fluorine atoms in the HOMO and LUMO are the main reason why the 1Blu(HOMO LUMO) values hardly change by H-F substitution in acenes.

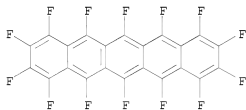
IT 646533-88-2, Perfluoropentacene

RL: PRP (Properties)

(electron-phonon interactions in photoinduced excited electronic states in fluoroacenes)

RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN

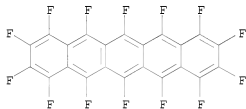
ACCESSION NUMBER: 2005:599413 CAPLUS

DOCUMENT NUMBER: 143:239497

TITLE: Organic thin-film transistors with high electron



AUTHOR(S): mobility based on perfluoropentacene  
 Inoue, Youji; Sakamoto, Youichi; Suzuki, Toshiyasu;  
 Kobayashi, Masafumi; Gao, Yuan; Tokito, Shizuo  
 CORPORATE SOURCE: NHK Science and Technical Research Laboratories,  
 Tokyo, 157-8510, Japan  
 SOURCE: Japanese Journal of Applied Physics, Part 1: Regular  
 Papers, Brief Communications & Review Papers (2005),  
 44(6A), 3663-3668  
 CODEN: JAPNDE  
 PUBLISHER: Japan Society of Applied Physics  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB We report on n-channel organic thin-film transistors (OTFTs) based on the  
 novel n-type organic semiconductor, perfluoropentacene. The transistor  
 exhibits excellent elec. characteristics, with a high electron mobility of  
 0.22 cm<sup>2</sup>/(V s) and a good current on/off ratio of 105. The electron  
 mobility is comparable to the hole mobility of a pentacene OTFT. By  
 combining the n-type perfluoropentacene and the p-type pentacene, we have  
 fabricated ambipolar OTFTs and complementary inverter circuits. The OTFTs  
 with heterostructures of the p- and n-type organic semiconductors can operate  
 as an ambipolar device with high electron and hole mobilities of 0.042 and  
 0.041 cm<sup>2</sup>/(V s). The complementary inverter using an n-channel  
 perfluoropentacene OTFT and a p-channel pentacene OTFT exhibits excellent  
 transfer characteristics with a voltage gain of 45. A complementary  
 inverter using the ambipolar OTFTs is also demonstrated.  
 IT 646533-88-2, Perfluoropentacene  
 RL: DEV (Device component use); PRP (Properties); USES (Uses)  
 (organic thin-film transistors with high electron mobility based on  
 perfluoropentacene)  
 RN 646533-88-2 CAPLUS  
 CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX  
 NAME)

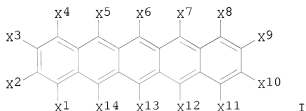


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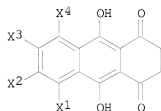
L4 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:409443 CAPLUS  
 DOCUMENT NUMBER: 142:463466  
 TITLE: Process for the preparation of fluorinated pentacene  
 derivatives  
 INVENTOR(S): Kobayashi, Masafumi; Omae, Osamu; Ohkubo, Kimitaka;  
 Gao, Yuan  
 PATENT ASSIGNEE(S): Kanto Denka Kogyo Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 59 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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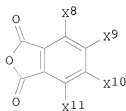
WO 2005042445	A2	20050512	WO 2004-JP16248	20041102
WO 2005042445	A3	20050714		
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US 20070083067	A1	20070412	US 2006-578259	20060504
PRIORITY APPLN. INFO.:			JP 2003-373970	A 20031104
			WO 2004-JP16248	W 20041102
OTHER SOURCE(S):	MARPAT 142:463466			
GI				



I



II



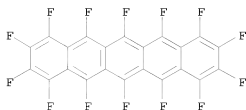
III

AB A process for the preparation of title compds. of formula I [wherein X1-X14 = F, H, (un)substituted alkyl, Ph, naphthyl, anthracenyl, naphthacenyl or pentacenyl; or X2X3 = cyclic ring; X9X10 = cyclic ring] via reaction of a compound of formula II with a compound of formula III is disclosed. For example, reaction of II (X1-X4 = F) with III (X8-X11 = F) gave 1,2,3,4,8,9,10,11-octafluoro-5,7,12,14-tetrahydroxypentacene-6,13-dione (IV) in 85% yield. Fluorination of IV with sulfur tetrafluoride gave 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetrafluoro-5,6,12,13,14-hexahydro-pentacene (V) in 40%. Defluorination of V with zinc provided the title compound I (X1-X14 = F) in 65% yield.

IT 646533-88-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of fluorinated pentacene derivs. via reaction of  
1,4-anthracenediones with 1,3-isobenzofurandiones)

RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



L4 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:1131758 CAPLUS

DOCUMENT NUMBER: 142:249827

TITLE: Effect of perfluorination on the charge-transport properties of organic semiconductors: density functional theory study of perfluorinated pentacene and sexithiophene

AUTHOR(S): Chen, Hsing-Yin; Chao, Ito

CORPORATE SOURCE: Institute of Chemistry, Academia Sinica, Taipei, 115, Taiwan

SOURCE: Chemical Physics Letters (2005), 401(4-6), 539-545

CODEN: CHPLBC; ISSN: 0009-2614

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB D. functional theory calcs. were carried out to investigate the effect of perfluorination on the reorganization energy ( $\lambda$ ) of charge-transport process. Fluorine substitution was found to increase the reorganization energy, disadvantageous for charge-transport. The enhancement of  $\lambda$  is attributed to addnl. contributions from the stretching of C-F bonds. On the other hand, perfluorination tends to increase electron affinity and ionization potential of compds., favoring for electron- rather than hole-transport in viewpoints of thermodyn. stability and injection barrier of charge. Based on these findings, valuable guidelines for the design of n-type materials with improved performance were proposed.

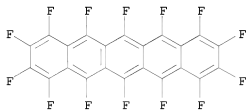
IT 646533-88-2, Perfluoropentacene

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)

(d. functional theory of effect of perfluorination on charge-transport properties of pentacene and sexithiophene)

RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetrafluoro- (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:577543 CAPLUS

DOCUMENT NUMBER: 141:260225

TITLE: The essential role of H-F substitution in the

electron-phonon interactions and electron transfer in the negatively charged acenes  
 AUTHOR(S): Kato, Takashi; Yamabe, Tokio  
 CORPORATE SOURCE: Fukui Institute for Fundamental Chemistry, Kyoto University, Sakyo-ku, Kyoto, 606-8103, Japan  
 SOURCE: Journal of Chemical Physics (2004), 121(5), 2356-2366  
 CODEN: JCPSA6; ISSN: 0021-9606  
 PUBLISHER: American Institute of Physics  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The single charge transfer through acenes, partially H-F substituted acenes, and fluoroacenes is discussed. The reorganization energies between the neutral mols. and the corresponding monoanions for partially H-F substituted acenes lie between those for acenes and fluoroacenes. The delocalization of the lowest unoccupied MOs (LUMO) by substituting hydrogen atoms by fluorine atoms with the highest electronegativity in every element is the main reason why the reorganization energy between the neutral mol. and the monoanion for partially H-F substituted acenes lies between those for acenes and fluoroacenes. This result implies that the neg. charged partially H-F substituted acenes would be better conductors with rapid electron transfer than the neg. charged fluoroacenes if we assume that the overlap of the LUMO between partially H-F substituted acenes is not significantly different from that between two neighboring fluoroacenes. The structures of the monoanions of acenes, fluoroacenes, and partially H-F substituted acenes are optimized under D2h geometry, and the Jahn-Teller effects in the monoanions of benzene and fluorobenzene are discussed. The vibration effect onto the charge transfer problem is also discussed. The C-C stretching modes around 1500 cm<sup>-1</sup> are the main modes converting the neutral mols. to the monoanions in acenes, fluoroacenes, and partially H-F substituted acenes. It can be confirmed from the calculational results that the C-C stretching modes around 1500 cm<sup>-1</sup> the most strongly couple to the LUMO in these mols. The main reason why the total electron-phonon coupling consts. (λLUMO) for the monoanions of acenes in which four outer hydrogen atoms are substituted by fluorine atoms are larger than those for the monoanions of acenes in which several inner hydrogen atoms are substituted by fluorine atoms is suggested. The relationships between the electron transfer and the electron-phonon interactions are discussed. The plot of the reorganization energies against the λLUMO values is found to be nearly linear. In view of these results, the relationships between the normal and superconducting states are briefly discussed.

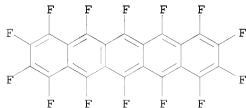
IT 646533-88-2 690975-12-3 756890-80-9  
 756897-54-8

RL: PRP (Properties)

(essential role of H-F substitution in electron-phonon interactions and electron transfer in neg. charged acenes)

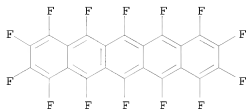
RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)

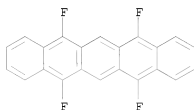


RN 690975-12-3 CAPLUS

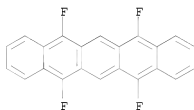
CN Pentacene, tetradecafluoro-, radical ion(1+) (9CI) (CA INDEX NAME)



RN 756890-80-9 CAPLUS  
 CN Pentacene, 5,7,12,14-tetrafluoro-, radical ion(1+) (9CI) (CA INDEX NAME)



RN 756897-54-8 CAPLUS  
 CN Pentacene, 5,7,12,14-tetrafluoro- (CA INDEX NAME)



REFERENCE COUNT: 99 THERE ARE 99 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:480070 CAPLUS

DOCUMENT NUMBER: 141:197895

TITLE: Perfluoropentacene: High-Performance p-n Junctions and Complementary Circuits with Pentacene  
 Sakamoto, Youichi; Suzuki, Toshiyasu; Kobayashi, Masafumi; Gao, Yuan; Fukai, Yasushi; Inoue, Youji; Sato, Fumio; Tokito, Shizuo

CORPORATE SOURCE: Institute for Molecular Science, Okazaki, 444-8787, Japan

SOURCE: Journal of the American Chemical Society (2004), 126(26), 8138-8140

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

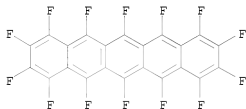
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors report the synthesis and characterization of perfluoropentacene as an n-type semiconductor for organic field-effect transistors (OFETs). Perfluoropentacene is a planar and crystalline material that adopts a herringbone structure as observed for pentacene. OFETs with

perfluoropentacene were constructed using top-contact geometry, and an electron mobility of 0.11 cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> was observed. Bipolar OFETs with perfluoropentacene and pentacene function at both neg. and pos. gate voltages. The improved p-n junctions are probably due to the similar d-spacings of both acenes. Complementary inverter circuits were fabricated, and the transfer characteristics exhibit a sharp inversion of the output signal with a high-voltage gain.

IT 646533-88-2P, Perfluoropentacene  
 RL: DEV (Device component use); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)  
 (perfluoropentacene: high-performance p-n junctions and complementary circuits with pentacene)  
 RN 646533-88-2 CAPLUS  
 CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:297458 CAPLUS

DOCUMENT NUMBER: 140:429323

TITLE: Inverse isotope effects and electron-phonon coupling in the positively charged deuterio- and fluoroacenes

AUTHOR(S): Kato, Takashi; Yamabe, Tokio

CORPORATE SOURCE: Fukui Institute for Fundamental Chemistry, Kyoto University, Sakyo-ku, Kyoto, 606-8103, Japan

SOURCE: Journal of Chemical Physics (2004), 120(16), 7659-7672  
 CODEN: JCPSA6; ISSN: 0021-9606

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Electron-phonon interactions in the monocations of deuterio- and fluoroacenes are studied and compared with those in the monocations of acenes and those in the monoanions of fluoroacenes. Because of the significant phase pattern difference between the highest occupied MOs (HOMO) and the lowest unoccupied MOs (LUMO), the frequency modes lower than 500 cm<sup>-1</sup> and the high-frequency modes around 1400 cm<sup>-1</sup> couple more strongly to the LUMO than to the HOMO, while the frequency modes around 500 cm<sup>-1</sup> and the frequency modes around 1600 cm<sup>-1</sup> couple more strongly to the HOMO than to the LUMO in fluoroacenes with D<sub>2h</sub> geometry. The total electron-phonon coupling consts. for the monocations (lHOMO) are estimated and compared with those for the monoanions (lLUMO) in deuterio- and fluoroacenes. The lHOMO values are estimated to be 0.418, 0.399, 0.301, 0.255, and 0.222 eV for C6F6 (1f), C10F8 (2f), C14F10 (3f), C18F12 (4f), and C22F14 (5f), resp. The lHOMO values are smaller than the lLUMO values in small fluoroacenes. But the lHOMO value decreases with an increase in mol. size less rapidly than the lLUMO value in fluoroacenes, and the lHOMO value of 0.074 eV is much larger than the lLUMO value of 0.009 eV in polyfluoroacene. The logarithmically averaged phonon frequencies for the monocations (oIn,HOMO) are estimated to be larger than those for the monoanions (oIn,LUMO) in fluoroacenes. This is because the C-C

stretching modes around 1600 cm<sup>-1</sup> couple most strongly to the HOMO, and those around 1400 cm<sup>-1</sup> couple the most strongly to the LUMO in fluoroacenes. The significant phase pattern difference between the HOMO and the LUMO is the main reason for the calculational results. The 1HOMO values increase much more significantly by H-F substitution than by H-D substitution in acenes. The possible inverse isotope effects in the electron-phonon interactions as a consequence of deuteration in the monocations of nanosized mols. are suggested.

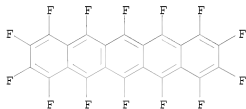
IT 690975-12-3

RL: PRP (Properties)

(inverse isotope effects and electron-phonon coupling in pos. charged deuterio- and fluoroacenes)

RN 690975-12-3 CAPLUS

CN Pentacene, tetradecafluoro-, radical ion(1+) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:898555 CAPLUS

DOCUMENT NUMBER: 140:118999

TITLE: Electron-phonon interactions in the monoanions of fluoroacenes

AUTHOR(S): Kato, Takashi; Yamabe, Tokio

CORPORATE SOURCE: Graduate School of Engineering, Department of Material Chemistry, Kyoto University, Sakyo-ku, Kyoto, 606-8501, Japan

SOURCE: Journal of Chemical Physics (2003), 119(21), 11318-11328

CODEN: JCPSA6; ISSN: 0021-9606

PUBLISHER: American Institute of Physics

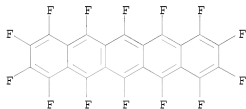
DOCUMENT TYPE: Journal

LANGUAGE: English

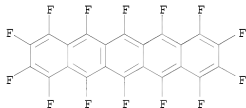
AB Electron-phonon interactions in the monoanions of fluoroacenes such as C6F6 (1f), C10F8 (2f), C14F10 (3f), C18F12 (4f), and C22F14 (5f) are studied, and compared with those in the monoanions of acenes and deuterio-acenes. The C-C stretching modes around 1500 cm<sup>-1</sup> the most strongly couple to the lowest unoccupied MOs (LUMO) in fluoroacenes. The estimated total electron-phonon coupling consts. (1LUMO) are 0.475, 0.473, 0.350, 0.273, and 0.215 eV for 1f, 2f, 3f, 4f, and 5f, resp. The 1LUMO values for fluoroacenes are much larger than those for acenes and deuterio-acenes. Possible superconducting transition temps. (Tcs) for the monoanions of deuterio-acenes and fluoroacenes are larger than those for the monoanions of acenes. The transition temperature (Tc) value increases much more significantly by H-F substitution than by H-D substitution in acenes. The 1LUMO and Tc values significantly decrease with an increase in mol. size from the monoanions of 1f to 5f. The logarithmically averaged phonon frequencies (ωln) do not significantly change with an increase in mol. size in the monoanions of fluoroacenes. The larger displacements of C atoms in the vibronic active modes in fluoroacenes than those in deuterio-acenes due to larger atomic mass of F than that of D, and the unchanged properties of the orbital patterns of the LUMO as a consequence

of H-F and H-D substitution in acenes, are the main reasons why the 1LUMO value increases much more significantly by H-F substitution than by H-D substitution, and the reason why the Tc value increases much more significantly by H-F substitution than by H-D substitution in acenes. The detailed properties of vibronic active modes and the electronic structures in the LUMO as well as the mol. wts. are closely related to the 1LUMO,  $\omega_{1n}$ , and Tc values in the monoanions of fluoroacenes, deuterioacenes, and acenes.

IT 646533-88-2  
 RL: PRP (Properties)  
 (carbon-carbon bond lengths in)  
 RN 646533-88-2 CAPLUS  
 CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



IT 645401-34-9  
 RL: PRP (Properties)  
 (electron-phonon interactions in)  
 RN 645401-34-9 CAPLUS  
 CN Pentacene, tetradecafluoro-, radical ion(1-) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 90 THERE ARE 90 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg		
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	ENTRY	SESSION
FULL ESTIMATED COST	110.44	289.01
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-16.00	-16.00

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DICTIONARY FILE UPDATES: 3 JUN 2008 HIGHEST RN 1025148-33-7

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<http://www.cas.org/support/stngen/stndoc/properties.html>

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	ENTRY	SESSION
FULL ESTIMATED COST	13.34	302.35
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-16.00

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STRUCTURE FILE UPDATES: 3 JUN 2008 HIGHEST RN 1025148-33-7  
DICTIONARY FILE UPDATES: 3 JUN 2008 HIGHEST RN 1025148-33-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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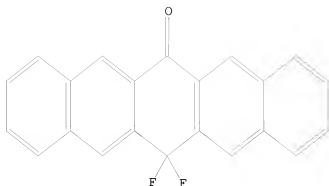
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L5 STRUCTURE UPLOADED

=> d 15

L5 HAS NO ANSWERS

L5 STR



Structure attributes must be viewed using STN Express query preparation.

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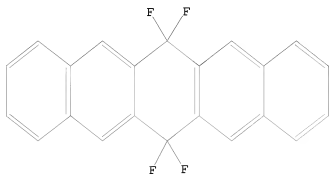
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L6 STRUCTURE UPLOADED

=> d 16

L6 HAS NO ANSWERS

L6 STR



Structure attributes must be viewed using STN Express query preparation.

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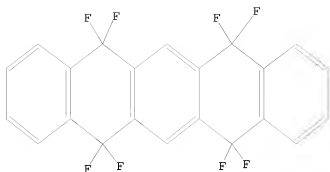
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L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR



Structure attributes must be viewed using STN Express query preparation.

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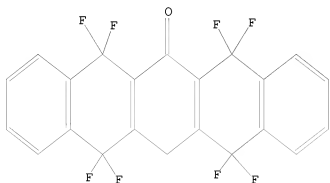
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L8 STRUCTURE UPLOADED

=> d 18

L8 HAS NO ANSWERS

L8 STR



Structure attributes must be viewed using STN Express query preparation.

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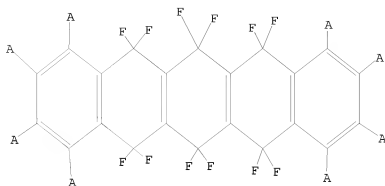
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L9 STRUCTURE UPLOADED

=> d 19

L9 HAS NO ANSWERS

L9 STR



Structure attributes must be viewed using STN Express query preparation.

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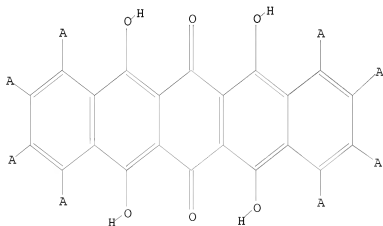
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L10 STRUCTURE UPLOADED

=> d l10

L10 HAS NO ANSWERS

L10 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l10 full

FULL SEARCH INITIATED 19:13:42 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 4771 TO ITERATE

100.0% PROCESSED 4771 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

L11 1 SEA SSS FUL L10

=> s 19 full

FULL SEARCH INITIATED 19:13:53 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 148 TO ITERATE

100.0% PROCESSED 148 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

L12 1 SEA SSS FUL L9

=> s 18 full  
FULL SEARCH INITIATED 19:14:00 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 29 TO ITERATE

100.0% PROCESSED 29 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

L13 1 SEA SSS FUL L8

=> s 17 full  
FULL SEARCH INITIATED 19:14:07 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 315 TO ITERATE

100.0% PROCESSED 315 ITERATIONS 2 ANSWERS  
SEARCH TIME: 00.00.01

L14 2 SEA SSS FUL L7

=> s 16 full  
FULL SEARCH INITIATED 19:14:15 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 173 TO ITERATE

100.0% PROCESSED 173 ITERATIONS 2 ANSWERS  
SEARCH TIME: 00.00.01

L15 2 SEA SSS FUL L6

=> s 15 full  
FULL SEARCH INITIATED 19:14:36 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 11 TO ITERATE

100.0% PROCESSED 11 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

L16 1 SEA SSS FUL L5

=> file caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	1071.08	1373.43
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-16.00

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FILE LAST UPDATED: 3 Jun 2008 (20080603/ED)

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<http://www.cas.org/legal/infopolicy.html>

=> s l11 or l12 or l13 or l14 or l15 or l16

3 L11  
4 L12  
1 L13  
1 L14  
3 L15  
1 L16  
6 L11 OR L12 OR L13 OR L14 OR L15 OR L16

L17

=> d l17 ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 6 ANSWERS - CONTINUE? Y/(N):y

L17 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on SIN

ACCESSION NUMBER: 2006:1304194 CAPLUS

DOCUMENT NUMBER: 146:52548

TITLE: Polyacene compound, its preparation, organic semiconductor element, and display device

INVENTOR(S): Nagata, Kazuto

PATENT ASSIGNEE(S): Asahi Kasei Corporation, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 30pp.

CODEN: JKXXXAF

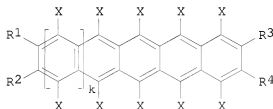
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006335719	A	20061214	JP 2005-164294	20050603
PRIORITY APPLN. INFO.:			JP 2005-164294	20050603
OTHER SOURCE(S):	MARPAT	146:52548		
GI				



I

AB Polyacene compound I (some of R1-4 are functional groups such as alkyl, alkenyl, alkynyl ester, alkyloxy, carbonyl, OH, etc., and others are H; some of Xs are F and others are H; k = 1-5) is claimed. The polyacene compound is prepared by (1) reducing polyacenequinone derivative to form hydroxypolyacene derivative, and (2) fluorinating and aromatizing it. Some other methods for preparing I are claimed. Crystalline organic semiconductor film

from I, transistor and display device using the film, a solution and ink containing I are also claimed. I shows good carrier transporting property, flexibility, solvent solubility, and oxidation resistance.

IT 916587-87-6P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(preparation of fluoropentacene compound)

RN 916587-87-6 CAPLUS

CN Pentacene, 6,6,13,13-tetrafluoro-2,3,9,10-tetrahexyl-6,13-dihydro- (CA INDEX NAME)



L17 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:1304192 CAPLUS

DOCUMENT NUMBER: 146:72036

TITLE: Preparation of polyacene compound and organic semiconductor element

INVENTOR(S): Nagata, Kazuto

PATENT ASSIGNEE(S): Asahi Kasei Corporation, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 21pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

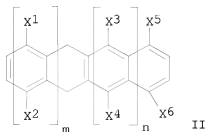
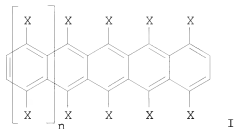
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

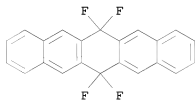
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006335720	A	20061214	JP 2005-164295	20050603
PRIORITY APPLN. INFO.:			JP 2005-164295	20050603
OTHER SOURCE(S):	MARPAT	146:72036		

GI



AB Polyacene compound I (some of Xs are F and others are H; k = 1-5) is prepared by (1) reacting polyacenequinone derivative II (X1-6 = H, F; m ≥ 2; m + n = 3-7) with a fluorination agent to form fluorinated polyacene derivative, and (2) defluorinating, dehydrogenating or dehydrofluorinating it. I is prepared by (1') reacting a hydroxypolyacene derivative with a fluorination agent to form fluorinated polyacene derivative, and (2). Some other methods for preparation I are also claimed. Crystalline organic semiconductor film from I, transistor and display device using the film, a solution and ink containing I are also claimed. I shows good carrier transporting property, flexibility, solvent solubility, and oxidation resistance.

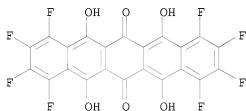
IT 851439-70-8P  
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of fluoropolyacene compound for organic semiconductive film)  
 RN 851439-70-8 CAPLUS  
 CN Pentacene, 6,6,13,13-tetrafluoro-6,13-dihydro- (CA INDEX NAME)



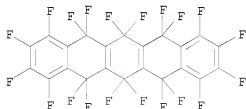
L17 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2006:88282 CAPLUS  
 DOCUMENT NUMBER: 145:177929  
 TITLE: Perfluoropentacene and Perfluorotetracene: Syntheses, Crystal Structures, and FET Characteristics  
 Sakamoto, Youichi; Suzuki, Toshiyasu; Kobayashi, Masafumi; Gao, Yuan; Inoue, Youji; Tokito, Shizuo  
 AUTHOR(S): Institute for Molecular Science, Myodaiji, Okazaki, Japan  
 CORPORATE SOURCE:



SOURCE: Molecular Crystals and Liquid Crystals (2006), 444,  
225-232  
CODEN: MCLCD8; ISSN: 1542-1406  
PUBLISHER: Taylor & Francis, Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The syntheses and FET characteristics of perfluoropentacene and  
perfluorotetracene are described. Both acenes are planar and crystalline  
materials that adopt p-stack structures with the short interplanar  
distances of 3.27 Å in perfluorotetracene and 3.21 Å in  
perfluoropentacene. The oxidation and reduction peak potentials of the  
perfluorinated acenes shift pos. compared with those of the corresponding  
acenes, suggesting that the HOMO and LUMO energies are diminished by  
fluorine substituents. Organic field-effect transistors (OFETs) with  
perfluoropentacene exhibit n-type semiconducting properties with high  
electron mobility of 0.22 cm<sup>2</sup>/V s.  
IT 851439-67-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(syntheses, crystal structures, and FET characteristics of  
perfluoropentacene and perfluorotetracene)  
RN 851439-67-3 CAPLUS  
CN 6,13-Pentacenedione, 1,2,3,4,8,9,10,11-octafluoro-5,7,12,14-tetrahydroxy-  
(CA INDEX NAME)



IT 738580-08-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(syntheses, crystal structures, and FET characteristics of  
perfluoropentacene and perfluorotetracene)  
RN 738580-08-0 CAPLUS  
CN Pentacene, 1,2,3,4,5,5,6,6,7,7,8,9,10,11,12,12,13,13,14,14-eicosafluoro-  
5,6,7,12,13,14-hexahydro- (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS ON STN  
ACCESSION NUMBER: 2005:903150 CAPLUS  
DOCUMENT NUMBER: 143:239906  
TITLE: Organic thin-film transistor, method for manufacturing  
same, and organic thin-film device

INVENTOR(S): Inoue, Youji; Tokito, Shizuo; Kobayashi, Masafumi;  
Gao, Yuan  
PATENT ASSIGNEE(S): Kanto Denka Kogyo Co., Ltd., Japan  
SOURCE: PCT Int. Appl., 43 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

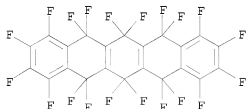
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005078816	A1	20050825	WO 2005-JP2495	20050217
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
JP 2005235923	A	20050902	JP 2004-41397	20040218
GB 2426125	A	20061115	GB 2006-16379	20050217
KR 2007009564	A	20070118	KR 2006-716513	20060817
US 20070194302	A1	20070823	US 2006-589800	20060817
PRIORITY APPLN. INFO.:			JP 2004-41397	A 20040218
			WO 2005-JP2495	W 20050217

AB Disclosed are an organic thin-film transistor with improved carrier mobility, a method for manufacturing an organic thin-film transistor, and an organic thin-film device comprising an organic thin-film transistor. Specifically disclosed is an organic thin-film transistor which comprises an organic semiconductor layer containing a fluorinated acene compound represented by the following formula:  $C_{4n+2}F_{2n+4}$  where n is an integer  $\geq 2$ . The fluorinated acene compound may preferably be a tetradecafluoropentacene or a dodecafluoronaphthalene.

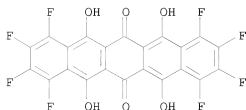
IT 738580-08-0P 851439-67-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(fluorinated acene thin-film transistor, method for manufacturing same, and organic thin-film device)

RN 738580-08-0 CAPLUS

CN Pentacene, 1,2,3,4,5,6,6,7,7,8,9,10,11,12,12,13,13,14,14-eicosafluoro-5,6,7,12,13,14-hexahydro- (CA INDEX NAME)



RN 851439-67-3 CAPLUS  
CN 6,13-Pentacenedione, 1,2,3,4,8,9,10,11-octafluoro-5,7,12,14-tetrahydroxy- (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on SIN

ACCESSION NUMBER: 2005:409443 CAPLUS

DOCUMENT NUMBER: 142:463466

TITLE: Process for the preparation of fluorinated pentacene derivatives

INVENTOR(S): Kobayashi, Masafumi; Omae, Osamu; Ohkubo, Kimitaka; Gao, Yuan

PATENT ASSIGNEE(S): Kanto Denka Kogyo Co., Ltd., Japan

SOURCE: PCT Int. Appl., 59 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005042445	A2	20050512	WO 2004-JP16248	20041102
WO 2005042445	A3	20050714		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

US 20070083067

A1 20070412

US 2006-578259

20060504

PRIORITY APPLN. INFO.:

JP 2003-373970

A 20031104

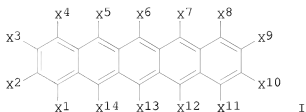
WO 2004-JP16248

W 20041102

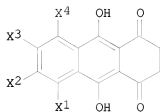
OTHER SOURCE(S):

MARPAT 142:463466

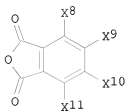
GI



I



II



III

AB A process for the preparation of title compds. of formula I [wherein X1-X14 = F, H, (un)substituted alkyl, Ph, naphthyl, anthracenyl, naphthacenyl or pentacenyl; or X2X3 = cyclic ring; X9X10 = cyclic ring] via reaction of a compound of formula II with a compound of formula III is disclosed. For example, reaction of II (X1-X4 = F) with III (X8-X11 = F) gave 1,2,3,4,8,9,10,11-octafluoro-5,7,12,14-tetrahydropentacene-6,13-dione (IV) in 85% yield. Fluorination of IV with sulfur tetrafluoride gave 1,2,3,4,5,5,6,6,7,7,8,9,10,11,12,12,13,13,14,14-eicosafluoro-5,6,7,12,13,14-hexahydro-pentacene (V) in 40%. Defluorination of V with zinc provided the title compound I (X1-X14 = F) in 65% yield.

IT 738580-08-0P 851439-67-3P 851439-70-8P

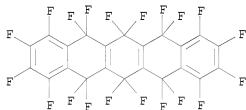
851439-72-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of fluorinated pentacene derivs. via reaction of 1,4-anthracenediones with 1,3-isobenzofurandiones)

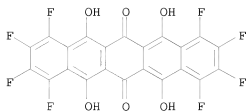
RN 738580-08-0 CAPLUS

CN Pentacene, 1,2,3,4,5,5,6,6,7,7,8,9,10,11,12,12,13,13,14,14-eicosafluoro-5,6,7,12,13,14-hexahydro- (CA INDEX NAME)

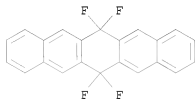


RN 851439-67-3 CAPLUS

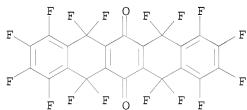
CN 6,13-Pentacenedione, 1,2,3,4,8,9,10,11-octafluoro-5,7,12,14-tetrahydroxy- (CA INDEX NAME)



RN 851439-70-8 CAPLUS  
 CN Pentacene, 6,6,13,13-tetrafluoro-6,13-dihydro- (CA INDEX NAME)



RN 851439-72-0 CAPLUS  
 CN 6,13-Pentacenedione, 1,2,3,4,5,5,7,7,8,9,10,11,12,12,14,14-hexadecafluoro-5,7,12,14-tetrahydro- (CA INDEX NAME)



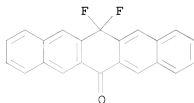
IT 851439-68-4P 851439-69-5P 851439-74-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of fluorinated pentacene derivs. via reaction of  
 1,4-anthracenediones with 1,3-isobenzofurandiones)  
 RN 851439-68-4 CAPLUS  
 CN Pentacene, 5,5,6,7,7,12,12,13,14,14-decafluoro-5,7,12,14-tetrahydro- (CA INDEX NAME)



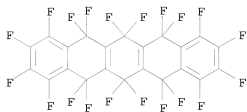
RN 851439-69-5 CAPLUS  
 CN Pentacene, 5,5,6,7,7,12,12,14,14-octafluoro-5,7,12,14-tetrahydro- (CA INDEX NAME)



RN 851439-74-2 CAPLUS  
 CN 6(13H)-Pentacenone, 13,13-difluoro- (CA INDEX NAME)



L17 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:480070 CAPLUS  
 DOCUMENT NUMBER: 141:197895  
 TITLE: Perfluoropentacene: High-Performance p-n Junctions and Complementary Circuits with Pentacene  
 AUTHOR(S): Sakamoto, Youichi; Suzuki, Toshiyasu; Kobayashi, Masafumi; Gao, Yuan; Fukai, Yasushi; Inoue, Youji; Sato, Fumio; Tokito, Shizuo  
 CORPORATE SOURCE: Institute for Molecular Science, Okazaki, 444-8787, Japan  
 SOURCE: Journal of the American Chemical Society (2004), 126(26), 8138-8140  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The authors report the synthesis and characterization of perfluoropentacene as an n-type semiconductor for organic field-effect transistors (OFETs). Perfluoropentacene is a planar and crystalline material that adopts a herringbone structure as observed for pentacene. OFETs with perfluoropentacene were constructed using top-contact geometry, and an electron mobility of 0.11 cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> was observed. Bipolar OFETs with perfluoropentacene and pentacene function at both neg. and pos. gate voltages. The improved p-n junctions are probably due to the similar d-spacings of both acenes. Complementary inverter circuits were fabricated, and the transfer characteristics exhibit a sharp inversion of the output signal with a high-voltage gain.  
 IT 738580-08-0P  
 RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
 (perfluoropentacene: high-performance p-n junctions and complementary circuits with pentacene)  
 RN 738580-08-0 CAPLUS  
 CN Pentacene, 1,2,3,4,5,5,6,6,7,7,8,9,10,11,12,12,13,13,14,14-eicosafluoro-5,6,7,12,13,14-hexahydro- (CA INDEX NAME)



REFERENCE COUNT:

24

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT